Institute for Scientific Computing Research

FY 1999 Annual Report

http://www.llnl.gov/casc/iscr

Lawrence Livermore National Laboratory
P.O. Box 808, L-561, Livermore, CA 94551

Center for Applied Scientific Computing

The University Relations Program (URP) encourages collaborative research between Lawrence Livermore National Laboratory (LLNL) and the University of California campuses. The Institute for Scientific Computing Research (ISCR) actively participates in such collaborative research, and this report details the Fiscal Year 1999 projects jointly served by URP and ISCR. For a full discussion of all URP projects in FY 1999, please request a copy of the URP FY 1999 Annual Report by contacting

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Contents

The Mission of the Institute for Scientific Computing Research

The Institute for Scientific Computing Research (ISCR) at Lawrence Livermore National Laboratory is jointly administered by the University Relations Program (URP) and the Center for Applied Scientific Computing (CASC), and this joint relationship expresses its mission. An extensively externally networked ISCR cost-effectively expands the level and scope of national computational science expertise available to the Laboratory, while streamlining the administrative burden that is unavoidable when bridging the Laboratory's internal computational research environment with that of the academic community.

As large-scale simulations on the parallel platforms of DOE's Accelerated Strategic Computing Initiative (ASCI) become increasingly important to the overall mission of LLNL, the role of the ISCR expands in importance, as well.

Relying primarily on nonpermanent staffing, the ISCR complements Laboratory research in areas of the computer and information sciences needed at the frontier of Laboratory missions. The ISCR works with CASC in being the "eyes and ears" of the Laboratory in the computer and information sciences, that is, in keeping the Laboratory aware of and connected to important advances. It also attempts to be "feet and hands" for the Laboratory by carrying those advances into the Laboratory and incorporating them into practice.

The ISCR has begun to and will increasingly provide continuing education opportunities for Laboratory personnel, in the form of on-site workshops taught by outside experts on novel software or hardware technologies.

The ISCR also seeks to influence the research community external to the Laboratory to pursue Laboratory-related interests, and to train the workforce that will be required by the Laboratory. Part of the performance of this function is interpreting to the external community appropriate (unclassified) aspects of the Laboratory's own contributions to the computer and information sciences — contributions that its unique mission and unique resources give it a unique opportunity and responsibility to make.

Of the three principal means of packaging scientific ideas for transfer — people, papers, and software — experience suggests that the most effective means is people. The programs of the ISCR are, therefore, people-intensive.

Finally, the ISCR, together with CASC, confers an organizational identity on the burgeoning computer and information sciences research activity at LLNL, and serves as a point of contact within the Laboratory for computer and information scientists from outside.

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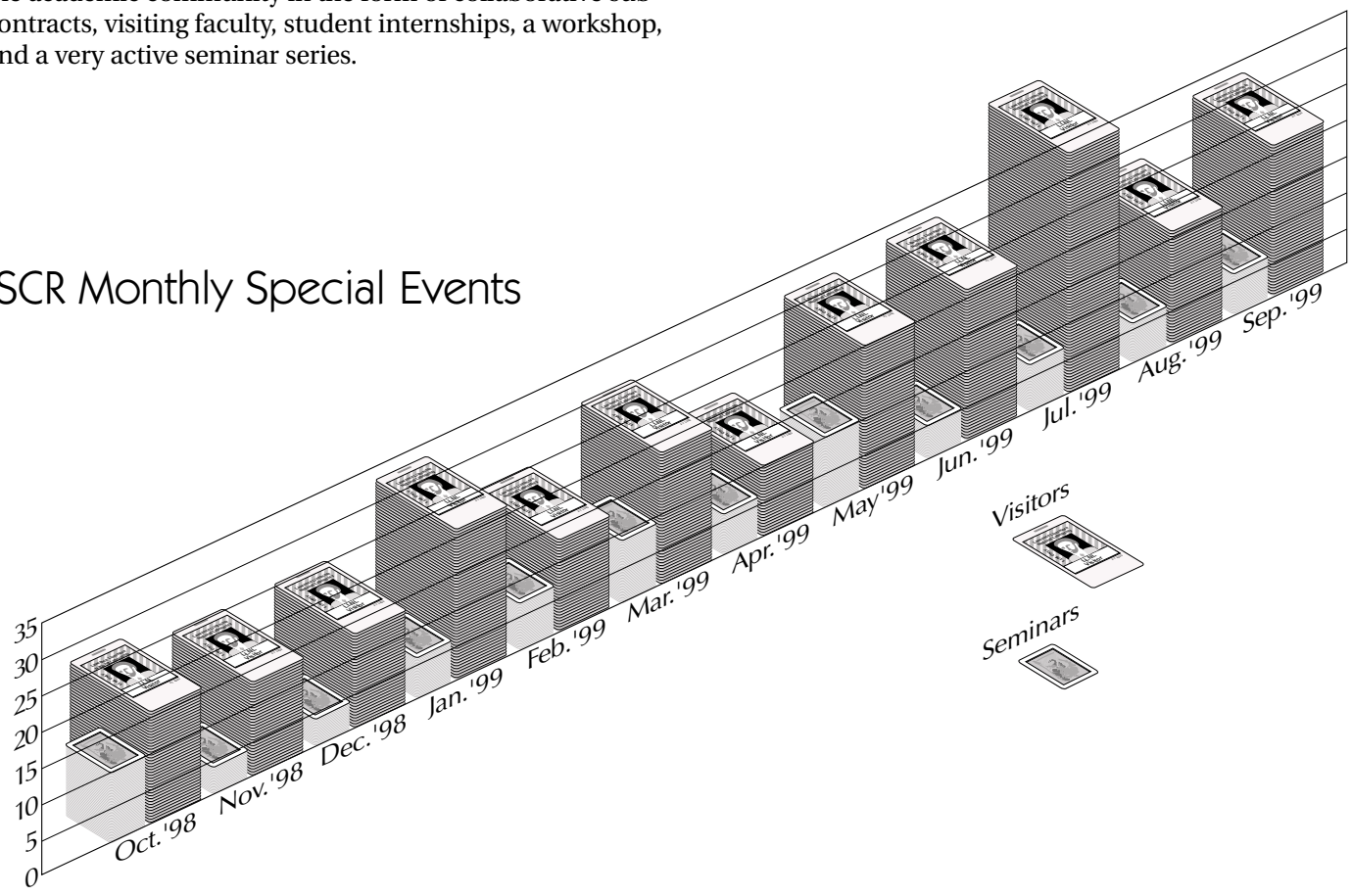
Large-scale scientific computation, and all of the disciplines that support it and help to validate it, have been placed at the focus of Lawrence Livermore National Laboratory by the Accelerated Strategic Computing Initiative (ASCI). The Laboratory operates the computer with the highest peak performance in the world and has undertaken some of the largest and most compute-intensive simulations ever performed. Computers at the architectural extremes, however, are notoriously difficult to use efficiently. Even such successes as the Laboratory's two Bell Prizes awarded in November 1999 only emphasize the need for much better ways of interacting with the results of large-scale simulations.

Advances in scientific computing research have, therefore, never been more vital to the core missions of the Laboratory than at present. Computational science is evolving so rapidly along every one of its research fronts that to remain on the leading edge, the Laboratory must engage researchers at many academic centers of excellence. In FY 1999, the Institute for Scientific Computing Research (ISCR) has expanded the Laboratory's bridge to the academic community in the form of collaborative subcontracts, visiting faculty, student internships, a workshop, and a very active seminar series.

ISCR research participants are integrated almost seamlessly with the Laboratory's Center for Applied Scientific Computing (CASC), which, in turn, addresses computational challenges arising throughout the Laboratory. Administratively, the ISCR flourishes under the Laboratory's University Relations Program (URP). Together with the other four Institutes of the URP, it must navigate a course that allows the Laboratory to benefit from academic exchanges while preserving national security. Although FY 1999 brought more than its share of challenges to the operation of an academic-like research enterprise within the context of a national security laboratory, the results declare the challenges well met and well worth the continued effort.

A change of administration for the ISCR occurred during FY 1999. Acting Director John Fitzgerald retired from LLNL in August after 35 years of service, including the last two at helm of the ISCR. David Keyes, who has been a regular visitor in conjunction with ASCI scalable algorithms research since October 1997, overlapped with John for three months and serves half-time as the new Acting Director.

ISCR Monthly Special Events



The pages of this report summarize the activities of the faculty members, post-doctoral researchers, students, and guests from industry and other laboratories who participated in LLNL's computational mission under the auspices of the ISCR during FY 1999.

Altogether, the ISCR hosted 215 visits from 167 different visitors, who gave a total of 80 seminars on site. The vast majority of the visitors were from academia, with 14% from industry and 8% from other laboratories. Visitors from outside of the United States comprised 7% of the total. The histogram on the previous page shows visitors and seminars as a function of the month of the fiscal year. It displays year-round activity, with higher than average on-site collaborations in the summer.

Most of the material of this annual report comes directly from the visitors and principal investigators of the projects being reported, who selected formats convenient for their purposes. We thank Alane Alchorn and Dan Moore for collecting over a hundred separate pieces of text that make up this report and producing an easily navigated and visually pleasing document.

We hope that you enjoy examining this report on the ISCR's diverse activities in FY 1999. For further information about the Institute, please contact us at the address below.

Inquiries regarding the ways in which you might enhance the ISCR Programs in FY 2000 or beyond are welcome.

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ISCR Fiscal Year 1999 in Review

FY 1999 Seminar Series (in reverse chronological order)

David O'Hallaron, Carnegie Mellon University	September 17, 1999
Linda Petzold, University of California, Santa Barbara	September 13, 1999
Jarmo Rantakokko, University of California, San Diego	September 10, 1999
Gundolf Haase, Johannes Kepler University, Linz	September 7, 1999
Ulrich Langer, Johannes Kepler University, Linz	September 7, 1999
Balakrishna Iyer, IBM Santa Theresa Labs	September 3, 1999
Ioana Banicescu, Mississippi State University	August 26, 1999
Valerio Pascucci, University of Texas, Austin	August 25, 1999
Howard Elman, University of Maryland	August 24, 1999
Joerg Meyer, University of California, Davis	August 20, 1999
Gerik Scheuermann, University of California, Davis	August 20, 1999
Petra Stapf, Daimler Chrysler AG	August 17, 1999
Andreas Stathopoulos, College of William and Mary	July 29, 1999
Gerard Meurant, Commissariat à l'énergie atomique	July 26, 1999
Fernando Reitich, University of Minnesota	July 23, 1999
Krister Ahlander, Uppsala University	July 16, 1999
Raytcho Lazarov, Texas A&M University	July 12, 1999
Calton Pu, Oregon Graduate Institute	July 9, 1999
Robert Haimes, Massachusetts Institute of Technology	July 7, 1999
Alexander Schweitzer, Universitaet Bonn	June 18, 1999
Robert Grossman, University of Illinois at Chicago	June 15, 1999
Donald Schwendeman, Rensselaer Polytechnic Institute	June 14, 1999
Jonathan Shewchuk, University of California, Berkeley	June 9, 1999
Gene Golub, Stanford University	May 27, 1999
Michael Minion, University of North Carolina	May 26, 1999
Pieter Hemker, Centrum voor Wiskunde en Informatica	May 24, 1999
Paul Barton, Massachusetts Institute of Technology	May 20, 1999
Ethan Miller, University of Maryland, Baltimore County	May 18, 1999
Chaitanya Baru, University of California, San Diego	May 14, 1999
Barton Miller, University of Wisconsin	May 10, 1999
David Muraki, New York University	May 7, 1999
Craig Douglas, University of Kentucky	May 4, 1999
Ivan Yotov, University of Pittsburgh	May 3, 1999
Luc Vincent, Xerox Corporation	April 29, 1999
Matthew O'Keefe, University of Minnesota	April 28, 1999
Dennis Gannon, NASA Ames and Indiana University	April 27, 1999
Alan Heirich, Compaq Tandem Laboratories	April 20, 1999
Marsha Berger, New York University	April 14, 1999
Robert Haimes, Massachusetts Institute of Technology	April 1, 1999

Larry Snyder, University of Washington	March 25, 1999
Mei-Ling Liu, California Polytechnic State University	March 22, 1999
Peter Beckman, Los Alamos National Laboratory	March 17, 1999
Dinesh Manocha, University of North Carolina, Chapel Hill	March 16, 1999
Robert Lowrie, Los Alamos National Laboratory	March 5, 1999
Beth Wingate, Los Alamos National Laboratory	March 4, 1999
Andrea Malagoli, University of Chicago	March 4, 1999
Andy Wathen, Oxford University	March 3, 1999
Dimitri Mavriplis, NASA Langley Research Center	February 25, 1999
Anders Petersson, Chalmers University of Technology	February 23, 1999
Ronald DeVore, University of South Carolina	February 19, 1999
Paul Hovland, Argonne National Laboratory	February 10, 1999
James Bramble, Texas A&M University	February 9, 1999
Cheryl Fillekes, Doyle Bouzaid Sailmakers, New Zealand	February 8, 1999
Petri Fast, New York University	February 1, 1999
Yelena Yesha, University of Maryland and NASA Goddard	January 28, 1999
Lou Kondic, Duke University	January 25, 1999
Richard Ewing, Texas A&M University	January 14, 1999
Calvin Ribbens, Virginia Polytechnic Institute and State University	January 12, 1999
Joseph Pasciak, Texas A&M University	January 11, 1999
Hanan Samet, University of Maryland	January 8, 1999
Samuel Uselton, MRJ Technology Solutions	December 18, 1998
Heinz-Otto Kreiss, University of California, Los Angeles	December 15, 1998
Alex Pothen, Old Dominion University	December 11, 1998
Michael J. Holst, University of California, San Diego	December 10, 1998
David M. Cooper, Lawrence Livermore National Laboratory	November 24, 1998
Gail Carpenter, Boston University	November 6, 1998
George Karypis, University of Minnesota	November 5, 1998
Sergei Nepomnyaschikh, Russian Academy of Sciences	November 4, 1998
Roy Hemker, University of California, Los Angeles	October 29, 1998
Wray Buntine, Ultimode Systems, LLC and UC Berkeley	October 22, 1998
E. Tina Cheng, University of California, Davis	October 20, 1998
Ramdas Ram-Mohan, Worcester Polytechnic Institute	October 19, 1998
Roger Wets, University of California, Davis	October 16, 1998
Glen Niebur, University of California, Berkeley	October 13, 1998
Charles Hansen, University of Utah	October 12, 1998
Mark Adams, University of California, Berkeley	October 6, 1998
Justin Wan, University of California, Los Angeles	October 5, 1998
Elmer Lewis, Northwestern University	October 1, 1998

Visiting Faculty, Guests, Consultants, and Researchers

Visiting and Collaborating Professors

Jack Dongarra, University of Tennessee
Michael Holst, University of California, San Diego
David Keyes, Old Dominion University
Raytcho Lazarov, Texas A&M University
Cal Ribbens, Virginia Polytechnic Institute and State University
Jinchao Xu, Pennsylvania State University
Ytha Yu, California State University, Hayward

Participating Guests

Mark Adams, University of California, Berkeley
Marsha Berger, New York University
Marian Brezina, University of Colorado
George Byrne, Illinios Institute of Technology
David Dean, University of Colorado
John Fitzgerald, Lawrence Livermore National Laboratory (retired)
Kyle Gallivan, Florida State University
Bernd Hamann, University of California, Davis
Stanley Johnson, Lehigh University
Falko Kuester, University of California, Davis
Martin Lades, Gene Trace
David Larson, Bay Area Research Corporation
Andrea Malagoli, University of Chicago
Michael Minion, University of North Carolina
Joseph Pasciak, Texas A&M University
Elbridge Gerry Puckett, University of California, Davis
John Rice, University of California, Berkeley
Yousef Saad, University of Minnesota
Paul Saylor, University of Illinois
Jeffrey Scroggs, North Carolina State University
Daniel Wake, TMA, Inc.

Consultants

Nabil Adams, Rutgers University
Berni Alder, University of California, Professor Emeritus
Randolph Bank, University of California, San Diego
Leo Breiman, University of California, Berkeley
Harry Dwyer, University of California, Davis

Consultants (continued)

Anne Greenbaum, University of Washington
Chuck Hansen, University of Utah
David Keyes, Old Dominion University
Heinz-Otto Kreiss, University of California, Los Angeles
Thomas Manteuffel, University of Colorado
Stephen McCormick, University of Colorado
Linda Petzold, University of California, Santa Barbara
Steve Schaffer, New Mexico Institute of Technology
Homer Walker, Worcester Polytechnic Institute

Postdoctoral Researchers

Erick Cantú-Paz
Petri Fast
Raymond Fellers II
Imola Fodor
Barry Lee
Brian J. Miller
Thomas Rutaganira
Leonid Tsap

University Collaborative Research Program Subcontractors

Scott Baden, University of California, San Diego
Abdul Barakat, University of California, Davis
Jackson Beatty, University of Califonia, Los Angeles
John Dawson, University of California, Los Angeles
Viktor Decyk, University of California, Los Angeles
Roy Hemker, University of California, Los Angeles
Warren Mori, University of California, Los Angeles
Linda Petzold, University of California, Santa Barbara
Fred Pollitz, University of California, Davis
Joachim Raeder, University of California, Los Angeles

LDRD Project Investigators

Peter Brown, LLNL Center for Applied Scientific Computing
Mark Duchaineau, LLNL Center for Applied Scientific Computing
Chandrika Kamath, LLNL Center for Applied Scientific Computing

Students and Faculty

Department of Applied Science Faculty

Nelson Max
Garry Rodrigue

Department of Applied Science Students

Henry J. Alme
Paul Covello
Rebecca Mattson Darlington
Joseph Koning
Daniel Laney
Sean Lehman
David Miller
Tim Pierce
Jonathan Rochez
Subhasis Saha
Jay Salmonson
Jay F. Thomas
Michael Everett Wickett

Visiting Students

Travis Austin, University of Colorado
Martin Bertram, University of California, Davis
Kathleen S. Bonnell, University of California, Davis
Thomas Brunner, University of Michigan
Timothy Chartier, University of Colorado
J. Kevin Durrenberger, California State University, Hayward
Daniel Ellis, Brigham Young University
Matt Giamporcaro, Boston University

Visiting Students (continued)

Ana Iontcheva, University of California, Davis
Mark Jeunnette, University of Chicago
Chisup Kim, Texas A&M University
Matthew Knepley, Purdue University
Eric LaMar, University of California, Davis
Gary Lee, University of California, Berkeley
Scott Morris, University of Utah
David Nault, University of Cincinnati
Jason Perry, University of Kentucky
Bobby Philip, University of Colorado
Alexandru Pomeranz, University of California, Davis
Lyn Reid, University of Washington
Kevin Scully, University of California, Irvine
Alex Tamasan, University of Washington
Heidi Thornquist, Rice University
Ben Tobin, Northern Arizona University
Stanimire Tomov, Texas A&M University
Kevin Vlack, University of Illinois, Urbana–Champaign
Christian Weiss, Technische Universitaet
Ludmil Zikatanov, Pennsylvania State University

National Physical Science Consortium (NPSC) Students

Lora Ballinger, University of Utah
Rachel Karchin, University of California, Santa Cruz
Imelda Kirby, University of Washington
Megan Thomas, University of California, Berkeley

Scalable Linear Solvers Workshop Leaders

Robert D. Falgout
Jinchao Xu